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Non-perturbative improvement of lattice QCD at large momenta

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ABSTRACT

We propose a method to improve lattice operators composed of Wilson fermions which allows the removal of all corrections of $O(a)$, including those proportional to the quark mass. It requires off-shell improvement of quark fields and composite operators, which is achieved by studying the behaviour of quark and gluon correlation functions at large momenta.

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1 Introduction

In present lattice computations an important source of errors is the finiteness of the lattice spacing, a. A systematic method for reducing discretization errors order by order in a was proposed by Symanzik [1] and developed by Lüscher and Weisz [2]. It consists of modifying the action and operators by "irrelevant" terms, chosen in such a way that the convergence to the continuum is accelerated. In the first implementations of this procedure, the improvement coefficients were computed in perturbation theory, leaving errors of $\mathrm{O}(ag_0^2)$ in physical quantities [3]. It turns out, however, that, for lattice spacings used in present simulations, one-loop perturbation theory is insufficiently precise for some quantities [4, 5], even when it is "tadpole improved" [6]. In refs. [7, 8] a method for determining the improvement coefficients beyond perturbation theory, based on the enforcement of Ward-Takahashi identities (WTI's) has been proposed and implemented, thus achieving full $O(a^2)$ improvement. This method allows one to determine the improved action and vector current for massive quarks (see also ref. [9]), but can only be applied to other operators, including the axial current, in the chiral limit. The reason for this limitation and a strategy to work outside the chiral limit valid in the case of on-shell matrix elements was discussed in ref. [10]. Vector and axial WTI's, possibly in conjunction with the use of unequal quark masses, have been employed to determine the coefficient of the term proportional to the mass in the normalization constants of certain quark bilinears [11, 12]. The question of $\mathrm{O}(am_q)$ corrections [2] is particularly significant for applications involving heavy quarks, where these terms may be large. Important examples in the phenomenology of B-mesons include the calculations of the leptonic decay constant f_B, the form factors of semileptonic B decays, the B-parameters and the amplitudes of the radiative decay $B \to K^*\gamma$.

In this paper we suggest an alternative method to extend operator improvement beyond the chiral limit, based on the consideration of the high momentum behaviour of quark correlators. The basic ingredient is the matching of lattice and continuum Green functions at large Euclidean momenta (or equivalently at short distances), where perturbation theory applies. An important property, crucial for our purposes, is that renormalized continuum correlators do not contain contact terms beyond those found in perturbation theory. This is a general consequence of the Callan-Symanzik equation, when applied at large momenta in an asymptotically free field theory. We stress that we aim only to remove errors proportional to a and do not attempt to work at arbitrary values of am_q, as in the program proposed in ref. [13]. In particular, after implementation of our proposal there will still remain errors proportional to $a^2m_q^2$.

Our method allows for the evaluation of the renormalization constants of divergent operators, such as the scalar and pseudoscalar densities. For a discussion of recent determinations of Z_P, Z_S and their ratio see ref. [14]. In principle this approach can be applied to composite operators of arbitrary dimension, though at the price of a very high proliferation of mixing operators, which may render the actual implementation of this scheme impractical.

[2] By m_q we mean some choice of physical quark mass. We do not need to pick a specific definition in this paper.

We wish to mention, as a side remark, an important limitation of the general idea of exploiting the large-momentum behaviour of correlators to renormalize composite operators non-perturbatively. The point is that for composite operators which can mix with lower dimensional ones, such as the octet part of the weak Hamiltonian, the strategy of killing at large momenta the "form factors" not allowed by chiral symmetry cannot be made to work. In fact lower dimensional operators may give rise to a large-momentum behaviour that cannot be distinguished from that due to the exchange of Goldstone bosons. For completeness we will briefly discuss this question in Appendix A.

An alternative method [15], which does not suffer from these limitations, is to measure on the lattice the behaviour of correlation functions in x-space in the region $a \ll |x| \ll \Lambda_{QCD}^{-1}$, where perturbation theory is reliable, and use the O.P.E. with perturbatively computed Wilson coefficients to fit this dependence. The parameters determined by the fitting procedure are the physical matrix elements of the (finite, renormalized) operators that appear in the O.P.E. In this way there is no need to know the expression of the renormalized operators in terms of the bare operators of the regularized (lattice) theory. The question here is whether the lattice is sufficiently fine-grained for the window $a \ll |x| \ll \Lambda_{QCD}^{-1}$ to exist. If this is the case, the method can be applied to a number of interesting cases, some of which are discussed in refs. [15] and [16].

The approach presented in this paper is a natural extension, valid up to $\mathrm{O}(a^2)$, of the method proposed in ref. [17], where the renormalization procedure is carried out in a non-perturbative way on correlators with external quarks and gluons. As discussed in ref. [17], such a procedure is expected to work if we can choose the virtuality of the external states, μ, at which the normalization is carried out, so as to satisfy $\Lambda_{\mathrm{QCD}} \ll \mu \ll 1/a$. Without improvement, the relative errors in matrix elements are of order am_q and $a\Lambda_{\mathrm{QCD}}$. In principle, our method is able to remove these errors and leave only corrections of $\mathrm{O}(a^2)$.

As has been said above, the condition $\Lambda_{\mathrm{QCD}} \ll \mu$ is required so that one can use perturbation theory to relate matrix elements renormalized on the lattice to those computed in standard continuum schemes. We wish to stress that, in principle, we can relax this constraint by using a sequence of lattices of decreasing a and correspondingly decreasing physical volumes. The idea is to determine the normalization constants by imposing renormalization conditions on a lattice with a very small lattice spacing. On such a fine-grained lattice large values of μ are allowed, but the smallness of the physical volume precludes the possibility of reliably computing hadronic correlation functions. It is therefore necessary to determine the corresponding normalization constants for the larger, but coarser, lattice on which the physical matrix elements are finally computed. This is achieved by increasing the lattice spacing a and matching the normalization constants at fixed μ, and successively decreasing μ and matching at fixed a. The procedure is repeated until the required value of a is reached. This method, which has been proposed within the context of the Schrödinger functional in ref. [7], could be applied also here. A first attempt in this direction has been made recently [18].

Our approach requires fixing the gauge, a procedure usually afflicted by Gribov ambigui-

ties [19] [3]. However, in the large-momentum region, where correlators are well described by perturbation theory, these ambiguities vanish asymptotically. Gauge fixing does however, introduce a further complication. When we evaluate correlators of gauge invariant operators with external quark and gluon fields, we need, in general, to include mixing with gauge non-invariant operators. The form of the latter is restricted by BRST symmetry [22, 23]. For flavour non-singlet quark bilinears, these restrictions are sufficient to forbid the appearance of gauge non-invariant terms until $O(a^2)$. For higher dimension operators, such as the four-fermion operators in the effective weak Hamiltonian, gauge non-invariant operators should be considered even at $O(a^0)$. The investigation of the consequences of BRST symmetry for the evaluation of Green functions of gauge-invariant operators between off-shell quark and gluon states is one of the principal goals of this paper. Our conclusions and the implications for the improvement of lattice actions and operators are presented in Sec. 2 below.

The paper is organized as follows. In Sec. 2 we explain our strategy and apply it to the improvement of quark fields. In Sec. 3 we discuss the procedure to improve quark bilinears fully up to $O(a^2)$. Few conclusive comments can be found in Sec. 4. The paper ends with three Appendices. In Appendix A we discuss in a simple example why in presence of spontaneous chiral symmetry breaking it is not possible to renormalize non-perturbatively operators that can mix with lower dimensional operators by only looking at the high momentum behaviour of correlators. In Appendix B we give a simple argument to prove that in off-shell amplitudes BRST-symmetry does not forbid the mixing of gauge-invariant operators with gauge non-invariant ones, if the latter vanish by the equations of motion. In Appendix C we apply our off-shell improvement procedure to the quark propagator calculated at one-loop order in perturbation theory.

2 Strategy and implementation on bilinears

Following ref. [7], we recall the basic steps of the Symanzik improvement program for lattice QCD up to $O(a^2)$. We will refer to the standard Wilson formulation of the theory. The improvement of the spectrum can be accomplished by adding the SW-Clover operator to the lattice QCD action with a coefficient determined using suitable WTI's identities for the axial current. This coefficient is a function of g_0^2, and has been determined non-perturbatively for several values of g_0^2 using numerical simulations [8]. The improvement of the action is not sufficient to remove $O(a)$ terms from correlation functions [2, 3]. To achieve this result one must also improve the relevant operators, by adding to them terms of three kinds [4]:

(a) Operators which vanish by the equations of motion, which can be either gauge invariant or non-invariant. They give rise only to contact terms, and thus do not affect the long-

[3] For recent progress on this issue see refs. [20, 21].

[4] This classification was introduced in the study of renormalization of gauge invariant operators, which requires, in general, operators of all three types [22] [23]. The classification applies as well for improvement, since the allowed operators are restricted by the same type of symmetries relevant for mixing.

distance properties of correlators.

(b) Gauge non-invariant, but BRST invariant, operators, which also do not contribute to physical amplitudes.

(c) Gauge-invariant operators which do not vanish by the equations of motion. These are needed to cancel discretization errors proportional to a in physical amplitudes.

Within the approach of ref. [7], by working in the chiral limit, one is able to improve operators by using only physical matrix elements. Improvement of composite operators in on-shell matrix elements was extended beyond the chiral limit in ref. [10] (see also refs. [11, 12]). In both cases only terms of type (c) are required. Here we need to consider all three types of terms.

The idea developed in this paper is to construct finite operators with well defined chiral transformation properties by matching lattice and continuum correlators in the region of large Euclidean momenta where perturbation theory applies. This is most easily done by requiring the vanishing of chirality-violating form factors in correlation functions in which the operator is inserted together with external quark and/or gluon (and possibly ghost) legs with large virtualities. This procedure is justified by the following two observations. First, at large momenta renormalized perturbation theory becomes chirally invariant (note that: i) explicit chiral symmetry breaking effects induced by the regularization can be reabsorbed by imposing the validity of the WTI's of chiral symmetry and ii) violations from the non-vanishing of quark masses disappear at large momenta). Secondly, contributions due to the spontaneous breaking of chiral symmetry, which are absent in perturbation theory, die off at large momenta. So the magnitude of both effects (which come from both perturbative and non-perturbative violations of chirality) decreases as we go deeper into the Euclidean region. As discussed in Appendix A, the argument cannot be applied to determine the mixing coefficients of lower dimensional operators.

In the following we consider correlation functions of elementary fields and multiplicatively renormalizable operators. They have, in general, non-vanishing anomalous dimensions. To discuss the improvement of such operators in a systematic way, one must first multiply them by appropriate renormalization constants so that they have a finite continuum limit. One can then speed up the approach to the continuum limit by adding further operators of $\mathrm{O}(a)$, and by allowing the normalization constants of fields and operators to depend on am_q. Thus, to the order at which we work, all the Z-factors we introduce will depend linearly on am_q. We do not, however, exhibit this dependence explicitly – it is fixed automatically by the overall normalization conditions that will be imposed.

2.1 Lattice BRST symmetry

In order to classify operators of type (b), i.e. gauge non-invariant operators which are BRST invariant, we need to know the form of the lattice BRST transformation. This is a simple generalization of the continuum transformation, as explained in ref. [24].

The lattice Landau gauge can be enforced by requiring that

$$G(U) = \sum_{n,\mu} \mathrm{Tr}(U_{n,\mu} + U^\dagger_{n,\mu}) \tag{1}$$

be locally maximized along a gauge orbit. This is equivalent to imposing, at each site n, and for each color a,

$$0 = f^a_n(U) = \frac{\delta G(U^g)}{\delta \omega^a_n}\Big|_{\omega=0} = i \sum_\mu \mathrm{Tr}\left[t^a(U_{n,\mu} - U^\dagger_{n,\mu}) - t^a(U_{n-\mu,\mu} - U^\dagger_{n-\mu,\mu})\right] , \tag{2}$$

where ω^a_n parameterizes the gauge transformation at site n and $g_n = \exp(i\omega^a_n t^a)$. The condition (2) is the discretized version of $\partial_\mu A^a_\mu(x) = 0$. We can implement the lattice Landau gauge in the functional integral in the standard way by adding to the action gauge fixing and ghost terms of the form

$$\mathcal{S}_{gf} = a^4 \sum_n \left[\frac{1}{2}\alpha\lambda^a_n\lambda^a_n + i\lambda^a_n f^a_n(U) + \sum_{n'} \bar{c}^a_n \frac{\delta f^a_n(U^g)}{\delta\omega^b_{n'}}\Big|_{\omega=0} c^b_{n'}\right] . \tag{3}$$

In eq. (3) c and $\bar{c}$ are ghost and anti-ghost fields, while λ is a Lagrange multiplier, all of which are defined on lattice sites. We obtain the lattice Landau gauge in the limit $\alpha \to 0$, for then the integral over λ^a_n sets $f^a_n = 0$.

There are, in general, many solutions to the gauge condition Eq. (2): this is the problem of Gribov copies [19, 25]. As mentioned in the introduction, we assume here the absence of copies for the gauge configurations which are responsible for the dominant contributions to correlation functions at large momenta.

The lattice action, $\mathcal{S}$, and the gauge-fixing action, $\mathcal{S}_{gf}$, are separately invariant under the appropriate BRST transformations. The latter are the lattice generalization of the continuum transformations. They are constructed by letting gauge and fermion fields be gauge transformed with a gauge matrix $g_n(c) = \exp(i\epsilon c^a_n t^a)$, where ϵ is a constant Grassmann parameter:

$$\epsilon\, \delta_{\mathrm{BRST}}\, q_n = g_n(c)q_n - q_n = i\epsilon c^a_n t^a q_n \tag{4}$$

$$\epsilon\, \delta_{\mathrm{BRST}}\, \overline{q}_n = -i\overline{q}_n \epsilon c^a_n t^a \tag{5}$$

$$\epsilon\, \delta_{\mathrm{BRST}}\, U_{n,\mu} = i\epsilon\left(c^a_n t^a U_{n,\mu} - U_{n,\mu} t^a c^a_{n+\mu}\right) . \tag{6}$$

Note that higher order terms vanish since $\epsilon^2 = 0$. The other fields transform in the usual way, i.e.

$$\delta_{\mathrm{BRST}}\, c^a_n = -\frac{1}{2} f_{abc} c^b_n c^c_n , \quad \delta_{\mathrm{BRST}}\, \bar{c}^a_n = \lambda^a_n , \quad \delta_{\mathrm{BRST}}\, \lambda^a_n = 0 . \tag{7}$$

The lattice BRST transformation is nilpotent, like its continuum counterpart.

The full action is also invariant under the anti-ghost shift symmetry, $\bar{c}^a_n \to \bar{c}^a_n + \mathrm{const}$. This symmetry is also very useful in restricting the form of improved operators.

2.2 Improvement of the action

The Wilson fermion action is improved by the addition of the SW operator,

$$\mathcal{S} = \mathcal{S}_{\rm gauge} + \mathcal{S}_{\rm Wilson} + a\int d^4x\ \mathcal{O}_{SW} \tag{8}$$

$$\equiv \mathcal{S}_{\rm gauge} + \int d^4x\ \overline{q}(\overrightarrow{\not{D}} + m_0)q\,, \tag{9}$$

where

$$\mathcal{O}_{SW} = -\frac{i}{4}c_{SW}\ \sum_{\mu\nu}\overline{q}\sigma_{\mu\nu}F_{\mu\nu}q\,, \tag{10}$$

with $\sigma_{\mu\nu} = (i/2)[\gamma_\mu,\gamma_\nu]$. In Eq. (9), $\overrightarrow{\not{D}} + m_0$ is a shorthand for the entire lattice fermion operator. Here and in the following we use continuum notation to refer to lattice quantities. For physical quantities to approach their continuum values with deviations of only $\mathrm{O}(a^2)$, we need, in addition to choosing the correct value of c_{SW}, to adjust the bare gauge coupling g_0 and the bare mass m_0 appropriately, in a way which depends on the renormalized quark mass. This is discussed in detail in ref. [7], but will not concern us here, since we have in mind fixing $a(g_0)$ and m_0 using hadronic quantities, such as m_ρ and m_π.

There are two additional gauge invariant operators of dimension 5 which could, in principle, be added to the action. The first one is

$$\mathcal{S}_1' = am_0c_1'\int d^4x\,\overline{q}(\overrightarrow{\not{D}} + m_0)q\,, \tag{11}$$

but this can be immediately eliminated by rescaling the quark fields. The second one can be written in the form

$$\mathcal{S}_2' = 2ac_2'\int d^4x\,\overline{q}(\overrightarrow{\not{D}} + m_0)^2q \tag{12}$$

and thus vanishes by the equations of motion. Although it can be neglected for the computation of on-shell quantities, it gives rise to contact terms in correlators. Its contributions can, however, be reabsorbed by a suitable redefinition of the $\mathrm{O}(a)$ part of fundamental fields and operators, as discussed below. Consequently we do not include it in the action.

Finally, we must consider the possibility that gauge non-invariant operators may need to be added to the action in order to improve quark and gluon correlation functions. Any such operator should be invariant under both the lattice BRST symmetry and the anti-ghost shift symmetry, and also under global color transformations, lattice rotations and translations. In addition, it must have zero ghost number. Allowed terms thus have the form (again using continuum notation for lattice quantities)

$$\mathcal{S}_{GNI} = \int d^4x\,\delta_{\rm BRST}\left[\bar{c}^a\partial_\mu X^a_\mu\right]\,,\quad X^a_\mu = X^a_\mu(\partial_\nu\bar{c},c,A,\bar{q},q,\lambda)\,, \tag{13}$$

where the vector X^a_μ is a color octet with zero ghost number. The possibility of lowest dimension is $X^a_\mu = A^a_\mu$, with some choice for the lattice gauge field, A^a_μ. This leads, however,

to a term proportional to $\mathcal{S}_{gf}(\alpha = 0) + \mathrm{O}(a^2)$, which can be absorbed by rescaling λ and α. Improvement terms of $\mathrm{O}(a)$ would result from choices of an X^a_μ of dimension 2. There exist, however, no such operators, and therefore no possible gauge non-invariant improvement terms at $\mathrm{O}(a)$. At next order, by contrast, there exist a number of possibilities, e.g. $X^a_\mu = \overline{q}\gamma_\mu t^a q$ or $X^a_\mu = f_{abc}c^b\partial_\mu \bar{c}^c$.

2.3 Improvement of quark fields

To improve quark fields to $\mathrm{O}(a^2)$ we must add all possible operators of dimension 5/2 which are allowed by the unbroken lattice symmetries. In particular, these operators must have the same properties as the quark fields under global gauge transformations, rotations and flavour transformations, and must satisfy the same BRST identities. The bare operators having these properties are $\not{D}q$, $m_0 q$ and $\not{\partial}q$. The appearance of $\not{\partial}q$ is, at first sight, surprising since it transforms differently from the quark field q under local gauge transformations [and thus under BRST transformations, Eq. (4)]. Nevertheless, as we now explain, the non-linearity of BRST symmetry does not exclude such an operator.

The constraints which follow from BRST symmetry can be obtained by requiring the improved operators to satisfy (up to $\mathrm{O}(a^2)$) the same identities that are satisfied by the continuum operators. The continuum identities take the form

$$\begin{aligned} 0 &= \langle \delta_{\mathrm{BRST}} \left[O_1(x_1) O_2(x_2) \ldots \right] \rangle \\ &= \langle \delta_{\mathrm{B}} [O_1(x_1)] O_2(x_2) \ldots \rangle \pm \langle O_1(x_1) \delta_{\mathrm{B}} [O_2(x_2)] \ldots \rangle + \ldots \,, \end{aligned} \tag{14}$$

where O_i are local composite operators located at arbitrary positions. The choice of sign on the second line depends on whether O_i is bosonic or fermionic. From now on to lighten the notation we will use the abbreviation δ_{B} for δ_{BRST}. Note that for the identities to be non-trivial the product of operators being varied must have ghost number -1. The conditions on the lattice operators become

$$\langle [\widehat{\delta_{\mathrm{B}} O_1}] \widehat{O}_2 \ldots \rangle \pm \langle \widehat{O}_1 [\widehat{\delta_{\mathrm{B}} O_2}] \ldots \rangle + \ldots = \mathrm{O}(a^2) \,, \tag{15}$$

where $\widehat{O}_i$ and $[\widehat{\delta_{\mathrm{B}} O_i}]$ are, respectively, the improved lattice versions of the continuum operator and of its continuum BRST variation. For brevity, we have subsumed the site label into the definition of the operator. The expectation value is to be taken with respect to the improved lattice action.

Since the improvement of the action does not break the lattice BRST symmetry, one can derive analogous BRST identities directly on the lattice

$$\langle \delta_{\mathrm{B}} [\widehat{O}_1] \widehat{O}_2 \ldots \rangle \pm \langle \widehat{O}_1 \delta_{\mathrm{B}} [\widehat{O}_2] \ldots \rangle + \ldots = 0 \,, \tag{16}$$

where the variations are under the lattice transformations (4)–(7). These identities are of the required form (15) if

$$[\widehat{\delta_{\mathrm{B}} O_i}] = \delta_{\mathrm{B}} [\widehat{O}_i] + \mathrm{O}(a^2) \,. \tag{17}$$

In other words, the improved lattice version of the continuum BRST variation on the l.h.s. must equal (up to $O(a^2)$) the lattice BRST variation of the improved operator on the r.h.s.

We now discuss the consequences of the condition (17). Since lattice and continuum BRST symmetries take the same form, (17) is automatically satisfied up to $O(a)$. Eq. (17) is thus a constraint on the form of improvement terms.

Consider first a gauge-invariant operator composed of quark and gluon fields. For this the continuum BRST variation vanishes and the condition (17) simply becomes $\delta_{\rm B}[\widehat{O}_i] = O(a^2)$. In other words, the terms of $O(a)$ added to improve O_i should themselves be invariant under the lattice BRST transformation, with the exception of operators which vanish by the equations of motion. These do not need to be BRST invariant because they contribute only when the insertion points of two operators happen to coincide, in which case the constraint (17) must be applied to the resulting composite operator. We do not discuss this issue further since, as explained below, BRST non-invariant operators are not needed for $O(a^2)$ improvement.

For the case of a quark field the continuum BRST variation is non-vanishing and the condition (17) becomes

$$it^a\widehat{[c^a q]} = \delta_{\rm B}[\widehat{q}] + O(a^2)\,. \tag{18}$$

As noted above, symmetries other than BRST require that the improved quark field has the form

$$\widehat{q} = Z_q^{-1/2}\left[1 + ac'_q(\overrightarrow{\not D} + m_0) + ac_{\rm NGI}\,\not\partial\right] q\,. \tag{19}$$

Here Z_q contains an implicit dependence on the quark mass, and we have chosen to group $\overrightarrow{\not D}$ with m_0 since this combination gives only contact terms in correlation functions. From Eq. (4) the lattice BRST variation of the improved quark field is

$$\delta_{\rm B}[\widehat{q}] = Z_q^{-1/2} it^a\left\{c^a\left[1 + ac'_q(\overrightarrow{\not D} + m_0)\right] q + ac_{\rm NGI}\,\not\partial[c^a q]\right\}\,. \tag{20}$$

Thus, comparing (20) with (18) and using (19), we learn that

$$\widehat{[c^a q]} = c^a\widehat{q} + aZ_q^{-1/2} c_{\rm NGI}[\not\partial c^a] q\,. \tag{21}$$

Naively, we might have expected the second term to be absent, since the ghost field itself does not require improvement at $O(a)$. But in fact we have no *a priori* knowledge of how to improve the composite operator $c^a q$, and there is no inconsistency with having the additional term proportional to $c_{\rm NGI}$. We conclude that BRST symmetry does not forbid non gauge invariant improvement terms for the quark field. For completeness we note that the improved antiquark field takes the form

$$\widehat{\overline{q}} = Z_q^{-1/2}\,\overline{q}\left[1 + ac'_q(-\overleftarrow{\not D} + m_0) - ac_{\rm NGI}\,\overleftarrow{\not\partial}\right]\,. \tag{22}$$

Having determined the general form of the improved quark and antiquark fields, we now explain our method for determining non-perturbatively the improvement coefficients c'_q and $c_{\rm NGI}$ and the normalization factor, Z_q.

To the order in a at which we are working, Z_q has a linear dependence on the quark mass, while c'_q and $c_{\rm NGI}$ are mass independent. The improvement condition is that the lattice and continuum renormalized quark propagators, $\widehat{S}$ and S respectively, differ only at $\mathrm{O}(a^2)$, i.e.

$$\widehat{S}(p) = S(p) + \mathrm{O}(a^2)\,. \tag{23}$$

Here, the renormalized lattice quark propagator in momentum space is defined by

$$\widehat{S}(p) \equiv \int d^4x e^{-ip\cdot x} \widehat{S}(x)\,, \tag{24}$$

where

$$\begin{aligned} &\widehat{S}(x) \equiv \langle \widehat{q}(x)\overline{\widehat{q}}(0)\rangle \\ &= Z_q^{-1} \left\langle \left[1 + ac'_q(\overrightarrow{\not{D}} + m_0) + ac_{\rm NGI}\, \not{\partial}\right] q(0)\overline{q}(x) \left[1 + ac'_q(-\overleftarrow{\not{D}} + m_0) - ac_{\rm NGI}\, \overleftarrow{\not{\partial}}\right]\right\rangle\,. \end{aligned} \tag{25}$$

In the following, we denote the bare lattice quark propagator by S_L ($S_L(x) = \langle q(x)\overline{q}(0)\rangle$).

The continuum renormalized quark propagator has the decomposition

$$S(p) = i\Sigma_1(p^2)\, \not{p} + \Sigma_2(p^2) \tag{26}$$

with some choice of normalization condition, to be specified below. The large p^2 behaviour of Σ_1 and Σ_2 is determined by the renormalization group equation [26]. In particular, $\Sigma_1(p^2) \stackrel{p^2\to\infty}{\longrightarrow} 1/p^2$ up to computable logarithmic corrections, while, in the chiral limit, $\Sigma_2(p^2) \stackrel{p^2\to\infty}{\longrightarrow} \langle\overline{q}q\rangle/p^4$, again up to logarithms, where $\langle\overline{q}q\rangle$ is the usual order parameter for spontaneous chiral symmetry breaking. Away from the chiral limit, Σ_2 still vanishes at large p^2, but now decreases as m_q/p^2. As already indicated in Eq. (23), our improvement condition will be that the lattice propagator has the same asymptotic behaviour as the continuum one up to $\mathrm{O}(a^2)$.

The effect of the improvement terms can be seen by deriving the expression for the improved propagator in momentum space. One gets

$$\begin{aligned} \widehat{S}(p) &= Z_q^{-1}\left(S_L(p) + 2ac'_q + ac_{\rm NGI}\{i\not{p}, S_L(p)\} + \mathrm{O}(a^2)\right) &(27)\\ &= Z_q^{-1}\left(S_L(p) + 2ac'_q\right) + 2ac_{\rm NGI}\left[2i\not{p}\Sigma_2(p^2) - p^2\Sigma_1(p^2)\right] + \mathrm{O}(a^2)\,. &(28) \end{aligned}$$

In the second line we have used Eq. (26) to parametrize the form of the propagator. The term proportional to c'_q thus adds a constant to the propagator, corresponding to a delta-function contact term in position space. The contribution from the term proportional to $c_{\rm NGI}$ is more complicated. In the chiral limit, and for large p^2, we can ignore Σ_2, and the $c_{\rm NGI}$ term is proportional to $p^2\Sigma_1(p^2)$. As already noted, this combination varies only logarithmically with p^2. Thus, in the chiral limit, the effect of the two improvement terms is similar. In practice this leads to problems in separately determining the two coefficients c'_q and $c_{\rm NGI}$ [14]. Away from the chiral limit, the $c_{\rm NGI}$ term also contributes a mass-dependent renormalization of the coefficient of $\not{p}$.

From this analysis we thus expect that the unimproved lattice propagator does not decrease at large momenta, but instead contains a constant and a slowly varying term which must be cancelled by appropriate choices of c'_q and $c_{\rm NGI}$. c'_q and $c_{\rm NGI}$ are then determined by requiring that the improved propagator satisfies, for a range of asymptotic values of $|p|$, the condition

$$\mathrm{Tr}\widehat{S}(p) = 0\,, \tag{29}$$

where the trace is over spin and colour indices. As Z_q is just an overall factor in this condition, we do not need to know it in advance in order to determine c'_q and $c_{\rm NGI}$. The implementation of Eq. (29) requires that the asymptotic behaviour of the correlation function can be extracted in the region where $p^2 \ll 1/a^2$ to avoid distortions due to $\mathrm{O}(a^2)$ errors. The same caveat applies to the improvement of bilinear operators discussed below. Exploratory numerical studies of the condition (29) can be found in [14].

Assuming that we have fixed c'_q and $c_{\rm NGI}$ in the way we have described, we can determine Z_q, by imposing, for instance, the condition

$$-i\frac{1}{48}\sum_\rho \mathrm{Tr}\left(\gamma_\rho \frac{\partial}{\partial p_\rho}\widehat{S}^{-1}(p)\right)\Big|_{p^2=\mu^2} = 1\,. \tag{30}$$

In view of the above discussion it may be preferable to determine Z_q using the forward matrix element of the conserved lattice current on quark states [17]. We note that, while different definitions of the field renormalization Z_q are possible, the coefficients c'_q and $c_{\rm NGI}$ are completely fixed by the form of the action, and are functions only of g_0^2. This is why they are completely determined by the asymptotic behaviour of Σ_2.

We can now see why c'_2 can be set to zero in the action. The reason is that the term proportional to c'_2, eq. (12), can be removed (up to $\mathrm{O}(a^2)$) by performing the change of variables

$$q \to \left[1 + ac'_2(\overrightarrow{\not{D}} + m_0)\right] q\,, \qquad \overline{q} \to \overline{q}\left[1 + ac'_2(-\overleftarrow{\not{D}} + m_0)\right]\,. \tag{31}$$

The expressions for the improved quark fields in terms of the new variables retain the same form, Eqs. (19) and (22), but with a shifted improvement coefficient $c'_q \to c'_q - c'_2$. The Jacobian for the change of variables shifts the $1/g_0^2$ coefficient in front of the gluon action, by a function of c'_2 [whose expansion begins at $\mathrm{O}(c_2'^4)$]. Since we are determining c'_q and $a(g_0)$ non-perturbatively, these shifts do not concern us. Similar shifts occur in the improvement coefficients, c'_O, of other quark bilinears which we will introduce below.

We have implemented the off-shell improvement procedure described in this sector in perturbation theory, using the one-loop results of Ref. [27]. Details are given in Appendix C. We find that a one-loop calculation can only separately determine the tree-level values of c'_q and c_{NGI} (the results are $c'_q = -1/4$ and $c_{NGI} = 0$). At one-loop accuracy, only the linear combination $c'_q + c_{NGI}$ can be determined. Thus, at present, the separate one-loop corrections to c'_q and c_{NGI} are not known.

3 Improvement of bilinear quark operators

In this section we discuss the improvement of local gauge-invariant bilinears. We consider only flavour non-singlet bilinears, but we drop flavour indices because they are not necessary for our discussion. We introduce the following notation:

- The amputated vertex function is defined as in the continuum [5]

$$\langle p|O_\Gamma|p'\rangle_{\rm amp} = \widehat{S}(p)^{-1} G_\Gamma(p,p') \widehat{S}(p')^{-1}\,, \tag{32}$$

  where

$$G_\Gamma(p,p') = \int d^4x d^4y e^{-ip\cdot x + ip'\cdot y} \langle \widehat{q}(x) O_\Gamma(0) \widehat{\overline{q}}(y)\rangle\,. \tag{33}$$

  with $O_\Gamma(x) = \overline{q}(x)\Gamma q(x)$ and Γ a Dirac matrix. Note that O_Γ is defined in terms of bare quark and antiquark fields. We do not construct the operator using improved quark fields $\widehat{q}$, because these contain the gauge non-invariant improvement term proportional to $c_{\rm NGI}$ which in the end, as we shall see, does not appear in bilinears.

- Improvement of bilinears requires consideration of operators of the form

$$E_\Gamma = \overline{q}\left[\Gamma(\overrightarrow{\not{D}} + m_0) + (-\overleftarrow{\not{D}} + m_0)\Gamma\right] q\,. \tag{34}$$

  These operators vanish by the equations of motion and therefore only contribute contact terms when inserted in correlators.

It turns out that the improvement of bilinears up to $\mathrm{O}(a^2)$ does not require the addition of gauge non-invariant operators. This is because there are no such operators with the same quantum numbers as the bilinears, having dimension 4. In fact, as mentioned above, allowed gauge non-invariant operators are of two types: those vanishing by the equations of motion, which need not be BRST invariant, and BRST invariant operators, which need not vanish by the equations of motion. The former appear first at dimension 5, an example being

$$\widehat{\overline{q}}\left[\Gamma\gamma_\mu t^a A^a_\mu(\overrightarrow{\not{D}} + m_0) + (-\overleftarrow{\not{D}} + m_0) t^a A^a_\mu \gamma_\mu \Gamma\right] \widehat{q}\,. \tag{35}$$

The lowest dimension BRST invariant operator has, instead, dimension 6:

$$\delta_{\rm B}\left(\overline{q}[\Gamma,\gamma_\mu]t^a q \partial_\mu \bar{c}^a\right) = \overline{q}[\Gamma,\gamma_\mu]t^a q\left[\partial_\mu \lambda^a + f_{abd}(\partial_\mu \bar{c}^b)c^d\right]\,. \tag{36}$$

Our restriction to flavour non-singlet operators is crucial here. Improvement of flavour singlet bilinears requires, in general, gauge non-invariant operators of dimension 4. For example, for $\Gamma = 1$, one requires operators of the form appearing in the gauge-fixing action, $\mathcal{S}_{gf}$.

[5] In ref. [17] the amputated vertex function was denoted $\Lambda_{O_\Gamma}(p,p')$.

3.1 Pseudoscalar density

The renormalized improved pseudoscalar density has the general form

$$\widehat{P}(x) \equiv Z_P P(x)\,, \tag{37}$$

$$P(x) = [\overline{q}(x)\gamma_5 q(x) + ac'_P E_{\gamma_5}(x)]\ . \tag{38}$$

The form of the terms in the amputated vertex which are cancelled by an appropriate choice of c'_P can be found by considering the contribution proportional to c'_P itself. This can be obtained by calculating the contribution of E_{γ_5} to the vertex function G_P (see Eq. (33)), with the result [6]

$$ac'_P \left[\widehat{S}(p)\gamma_5 + \gamma_5 \widehat{S}(p')\right] + \mathrm{O}(a^2)\,. \tag{39}$$

After amputation, one finds

$$\langle p|ac'_P E_{\gamma_5}|p'\rangle_{\rm amp} = ac'_P \left[\gamma_5 \widehat{S}(p')^{-1} + \widehat{S}(p)^{-1}\gamma_5\right] + \mathrm{O}(a^2)\,. \tag{40}$$

For large p^2, p'^2 and $(p-p')^2$ we expect the continuum vertex function to approach its perturbative form, and thus that the only surviving form factor is that proportional to γ_5. Indeed, because of chiral symmetry, the form factor proportional to $\gamma_\mu\gamma_5$ vanishes in continuum perturbation theory when $m_q = 0$. If improvement were not implemented however, a contribution of $\mathrm{O}(a)$ proportional to $a(p-p')_\mu\gamma_\mu\gamma_5$ would survive, as can be seen by substituting $\widehat{S}(p)^{-1} \sim \not{p}$ into Eq. (40). This may be cancelled by tuning c'_P. One can thus determine c'_P by setting $p \neq p'$ and imposing the condition

$$\lim_{|p|,|p'|,|p-p'|\to\infty} \mathrm{Tr}\left(\gamma_\mu\gamma_5\langle p|P|p'\rangle_{\rm amp}\right) = 0\,. \tag{41}$$

An incorrect choice of c'_P would result in an $\mathrm{O}(a)$ contribution to this trace growing like p_μ. Eq. (41) is equivalent to determining c'_P from

$$-ac'_P = \lim_{|p|,|p'|,|p-p'|\to\infty} \frac{\mathrm{Tr}\left(\gamma_\mu\gamma_5\langle p|\overline{q}\gamma_5 q|p'\rangle_{\rm amp}\right)}{\mathrm{Tr}\left(\gamma_\mu\gamma_5\langle p|E_{\gamma_5}|p'\rangle_{\rm amp}\right)}\,, \tag{42}$$

which shows that the overall normalization of the operator need not be fixed before determining c'_P.

The normalization constant Z_P is logarithmically divergent as $a \to 0$, and should be fixed by a renormalization condition. A possible choice is

$$Z_P \frac{1}{12}\mathrm{Tr}\left(\gamma_5\langle p|P|p\rangle_{\rm amp}\right)\Big|_{p^2=\mu^2} = 1\,. \tag{43}$$

We note that it is necessary to determine c'_P before Z_P. The point is that Eq. (40) contains a term of $\mathrm{O}(a)$ which is proportional to γ_5, coming from the "mass term" in the inverse propagator, i.e. from the part of $\widehat{S}^{-1}$ proportional to the identity. Tuning c'_P thus changes the γ_5 form factor by terms of $\mathrm{O}(a)$, and so changes the resulting value of Z_P. Note also that an error in the determination of c'_P leads to an error in the $\mathrm{O}(a)$ part of Z_P that is proportional to am_q. Similar comments apply to other bilinears.

[6] We stress that G_P contains the insertion of the operator P and not $\widehat{P}$.

3.2 Vector Current

The improved vector current has the general form

$$\widehat{V}_\mu(x) = Z_V V_\mu(x)\,, \tag{44}$$

$$V_\mu(x) = \overline{q}(x)\gamma_\mu q(x) + ac_V \sum_\nu i\partial_\nu \left[\overline{q}(x)\sigma_{\mu\nu} q(x)\right] + ac'_V E_{\gamma_\mu}(x)\,. \tag{45}$$

In this case, improvement requires the determination of three constants, one more than for the pseudoscalar density. The new type of constant, c_V, is to be chosen to remove $\mathrm{O}(a)$ contributions to physical amplitudes in the chiral limit. It was introduced and discussed in ref. [7] and determined in refs. [12, 9]. The contribution proportional to c'_V is needed to cancel contact terms of $\mathrm{O}(a)$. Finally, the part of Z_V proportional to am_q (usually called b_V) should be chosen so that the vector current is normalized as in the continuum up to $\mathrm{O}(a^2)$. The normalization Z_V is not arbitrary, unlike that of the pseudoscalar density, but should be fixed so that the vector current satisfies the usual current algebra relations. Z_V is finite in the continuum limit.

To determine the improvement constants c_V and c'_V we use the fact that, for the vector current, the only continuum form factor which survives at large momenta is that proportional to γ_μ. The contribution of c'_V to the amputated vertex, $\langle p|V_\mu|p'\rangle_{\mathrm{amp}}$, is

$$ac'_V \left[\gamma_\mu \widehat{S}(p')^{-1} + \widehat{S}(p)^{-1}\gamma_\mu\right] + \mathrm{O}(a^2)\,, \tag{46}$$

which for large $|p|$, $|p'|$ and $|p-p'|$ is proportional to

$$ac'_V \left[\gamma_\mu \not{p}' + \not{p}\gamma_\mu\right] + \mathrm{O}(a^2) = ac'_V \left[(p+p')_\mu + i\sigma_{\mu\nu}(p-p')_\nu\right] + \mathrm{O}(a^2)\,. \tag{47}$$

The contribution of c_V, on the other hand, is asymptotically proportional to $\sigma_{\mu\nu}(p-p')_\nu$. In the unimproved current, therefore, contributions of $\mathrm{O}(a)$ proportional to the identity and to $\sigma_{\mu\nu}$ are not suppressed, and must be cancelled by tuning c_V and c'_V. We can determine c'_V separately by setting $p = p'$, since in this case the c_V term does not contribute, being proportional to a total divergence. To isolate the unwanted form factor we project onto the identity matrix, and impose the asymptotic condition

$$\lim_{|p|\to\infty} \mathrm{Tr}\left(\langle p|V_\mu|p\rangle_{\mathrm{amp}}\right) = 0\,. \tag{48}$$

Having determined c'_V, we then fix c_V by requiring that the tensor form factor is absent asymptotically, i.e.

$$\lim_{|p|,|p'|,|p-p'|\to\infty} \mathrm{Tr}\left(\sigma_{\mu\nu}\langle p|V_\mu|p'\rangle_{\mathrm{amp}}\right) = 0\,. \tag{49}$$

Here and in the following, there is no implied summation over repeated indices unless explicitly indicated. Since the tuning of c'_V affects both scalar and tensor form factors, it is necessary that the conditions (48) and (49) be applied in the specified order.

Finally, the normalization constant Z_V can be obtained by imposing the WTI

$$Z_V \sum_\mu \langle p|\widetilde{\partial}_\mu V_\mu|p'\rangle_{\rm amp} = \widehat{S}(p)^{-1} - \widehat{S}(p')^{-1}\,, \tag{50}$$

where $\widetilde{\partial}_\mu$ is the symmetric (improved) lattice derivative

$$\widetilde{\partial}_\mu f(x) = \frac{1}{2a}\left[f(x+a\widehat{\mu}) - f(x-a\widehat{\mu})\right]\,. \tag{51}$$

As discussed in ref. [17], this gives the same result as the condition

$$Z_V \frac{1}{12}{\rm Tr}\left(\gamma_\nu \langle p|V_\nu|p\rangle_{\rm amp}\right)\Big|_{p^2=\mu^2} = 1\,. \tag{52}$$

Note that, if we express all improved quark fields in terms of bare quark fields, using Eqs. (19) and (22), both sides of Eq. (50) will be proportional to Z_q. Thus we do not to need to know Z_q in order to determine Z_V using the WTI. The factors of Z_q simply ensure that each term in Eq. (50) remains finite in the continuum limit.

An alternative way of determining Z_V is to require that the charge of a particular hadron equals its physical value. In practice, this may be preferable to the methods described above, which are based on quark correlators, since determinations using hadronic states typically have smaller errors.

3.3 Axial Current

Improvement of the axial current is accomplished following similar steps to those needed for the vector current. The improved form of the axial current is

$$\begin{aligned}
\widehat{A}_\mu(x) &= Z_A A_\mu(x)\,, & (53)\\
A_\mu(x) &= \overline{q}(x)\gamma_\mu\gamma_5 q(x) + a c_A \partial_\mu\left[\overline{q}(x)\gamma_5 q(x)\right] + a c'_A E_{\gamma_\mu\gamma_5}(x)\,. & (54)
\end{aligned}$$

In this case, the contribution of $E_{\gamma_\mu\gamma_5}$ to the amputated vertex, $\langle p|A_\mu|p'\rangle_{\rm amp}$, is

$$a c'_A\left[\gamma_\mu\gamma_5\widehat{S}(p')^{-1} + \widehat{S}(p)^{-1}\gamma_\mu\gamma_5\right] + {\rm O}(a^2)\,. \tag{55}$$

The only form factor which must survive asymptotically in the continuum is that proportional to $\gamma_\mu\gamma_5$. We therefore first determine c'_A from the condition

$$\lim_{|p|\to\infty} {\rm Tr}\left(\sigma_{\mu\nu}\gamma_5\langle p|A_\mu|p\rangle_{\rm amp}\right) = 0 \tag{56}$$

and then fix c_A by imposing

$$\lim_{|p|,|p'|,|p-p'|\to\infty} {\rm Tr}\left(\gamma_5\langle p|A_\mu|p'\rangle_{\rm amp}\right) = 0\,. \tag{57}$$

Finally, the normalization constant Z_A can be determined by enforcing the WTI

$$Z_A\langle p|\sum_\mu \widetilde{\partial}_\mu A_\mu|p'\rangle_{\rm amp} - 2\widehat{m}_q Z_P\langle p|P|p'\rangle_{\rm amp} = -\left[\widehat{S}(p')^{-1}\gamma_5 + \gamma_5\widehat{S}(p)^{-1}\right]. \tag{58}$$

For $p = p'$ this identity fixes the value of $\widehat{m}_q$, since the first term on the l.h.s. vanishes. Here, $\widehat{m}_q$ is a possible definition of the renormalized quark mass, which is automatically improved to $\mathrm{O}(a^2)$, being determined from quantities that are already improved at this order. Note that the combination $\widehat{m}_q Z_P$ is determined unambiguously, but that, as in the continuum, the value of $\widehat{m}_q$ depends on the normalization condition chosen for Z_P. Having found $\widehat{m}_q$, Z_A can then be obtained by considering $p \neq p'$, and tracing Eq. (58) with $\gamma_\mu\gamma_5$. As for Z_V, the determinations of $\widehat{m}_q$ and Z_A do not require knowledge of Z_q.

3.4 Scalar and tensor bilinears

Finally, we briefly sketch the analysis for the scalar and tensor operators. The improved scalar density is

$$\widehat{S}(x) = Z_S S(x), \tag{59}$$
$$S(x) = \overline{q}(x)q(x) + ac'_S E_S(x). \tag{60}$$

We can fix c'_S from the condition

$$\lim_{|p|\to\infty} \mathrm{Tr}\left(\gamma_\mu\langle p|S|p\rangle_{\rm amp}\right) = 0 \tag{61}$$

and then determine Z_S by imposing

$$Z_S\frac{1}{12}\mathrm{Tr}\left(\langle p|S|p\rangle_{\rm amp}\right)\Big|_{p^2=\mu^2} = 1. \tag{62}$$

The improved tensor operator has the form

$$\widehat{T}_{\mu\nu}(x) = Z_T T_{\mu\nu}(x), \tag{63}$$
$$T_{\mu\nu}(x) = i\overline{q}(x)\sigma_{\mu\nu}q(x) + ac_T(\partial_\mu V_\nu - \partial_\nu V_\mu) + ac'_T E_{T_{\mu\nu}}(x), \tag{64}$$

where in V_μ, defined in Eq. (45), one does not need to include the $O(a)$ terms proportional to c_V and c'_V. We can obtain c'_T by requiring

$$\lim_{|p|\to\infty} \mathrm{Tr}\left(\gamma_\rho\gamma_5\langle p|T_{\mu\nu}|p\rangle_{\rm amp}\right) = 0, \tag{65}$$

where all Lorentz indices are different, and then determine c_T by enforcing the condition

$$\lim_{|p|,|p'|,|p-p'|\to\infty} \mathrm{Tr}\left(\gamma_\mu\langle p|T_{\mu\nu}|p'\rangle_{\rm amp}\right) = 0. \tag{66}$$

Finally, we can fix Z_T by imposing

$$Z_T\frac{1}{12}\mathrm{Tr}\left(\sigma_{\nu\rho}\langle p|T_{\nu\rho}|p\rangle_{\rm amp}\right)\Big|_{p^2=\mu^2} = 1. \tag{67}$$

4 Conclusions

We have presented a method for determining the off-shell improvement coefficients of gauge invariant bilinears in the massive case, using quark correlation functions. We stress that our ultimate interest is in the calculation of the coefficients necessary for the improvement of on-shell quantities, but that we might wish to use off-shell correlators as an intermediate step. A detailed numerical study will be necessary to determine whether the method is practical. The pilot study of ref. [14] suggests that it will be difficult to separate c'_q from c_{NGI}, in which case the method works only in the chiral limit.

The whole approach can be extended to the case of non-degenerate quark masses, which is relevant for heavy flavour phenomenology. The only change is in the form of the WTI's. For the axial WTI, $2\widehat{m}_q$ should be replaced by $\widehat{m}_1 + \widehat{m}_2$, while for the vector identity, a term proportional to the mass difference should be added.

The approach can also be extended to deal with more complicated composite operators, such as four-quark operators relevant to study the effective weak Hamiltonian, though the number of operators which must be included may render the procedure impractical.

We stress again, however, that our approach fails, in general, for operators which can mix with lower dimensional ones (such as the octet part of the weak Hamiltonian). In this situation, lower dimensional operators may give rise in correlators to a large momentum behaviour that cannot be distinguished, and thus disentangled, from that coming from the exchange of Goldstone bosons in correlators with the insertion of the original operator.

Appendix A

In this Appendix we want to explain in a simple example why, in presence of spontaneous breaking of chiral symmetry, it may not be possible to fix non-perturbatively all the coefficients of the mixing of lower dimensional operators with higher dimensional ones by simply looking at the high momentum behaviour of correlators. The reason is that correlators with the insertion of lower dimensional operators may turn out to have the same high momentum behaviour as that coming from contributions due to the exchange of Goldstone bosons to (some of the) correlators in which the original operator is inserted.

To prove this statement let us consider the correlator [7]

$$G_d^A(p,p') \equiv \int d^4x d^4y e^{-ipx+ip'y} \langle \delta_A\Big(\bar{q}(y)q(x)O_d(0)\Big)\rangle \,, \tag{68}$$

where O_d is an operator of dimension d and $\delta_A(O)$ represents the axial variation of the operator O. A simple dimensional counting shows that the asymptotic scaling behaviour of

[7] As in the rest of the paper also in this Appendix to simplify notations we will neglect flavour indices.

$G_d^A(p,p')$ for large p and p' is given by the formula

$$G_d(\lambda p, \lambda p') \underset{\lambda\to\infty}{\sim} \lambda^{d-5}\,. \tag{69}$$

A similar analysis for the Green function

$$G_d^m(p,p') \equiv m \int d^4x\, d^4y\, d^4z\, e^{-ipx+ip'y} \langle \bar{q}(z)\gamma_5 q(z) \bar{q}(y) q(x) O_d(0)\rangle\,, \tag{70}$$

in which the operator $P = \bar{q}\gamma_5 q$ is inserted together with O_d, gives

$$G_d^m(\lambda p, \lambda p') \underset{\lambda\to\infty}{\sim} \lambda^{d-6}\,. \tag{71}$$

Suppose now we are interested in the case of the mixing of an operator of dimension 6 (like the octet part of the effective weak Hamiltonian) with an operator of dimension 3 (like $\bar{q}\gamma_5 q$ or $\bar{q}q$). From the scaling behaviours (69) and (71) we immediately conclude that, in the absence of a massless pion, everything works fine, because at large momenta

1) the contribution of the correlator G_d^m to the relevant axial WTI is subleading with respect to that coming from G_d^A both for $d = 6$ and $d = 3$;

2) correlators with inserted operators of dimension 6 and 3 have well separated asymptotic behaviours.

In this circumstance the unwanted contributions (i.e. those corresponding to $d = 3$ in the above scaling laws) can be isolated in the various correlators and set to zero by appropriately choosing the mixing coefficients at our disposal.

The problem arises if chirality is spontaneously broken, because in the chiral limit the pion contributes to G_6^m a term

$$\begin{aligned} G_6^m(p,p')\Big|_{pion} &= f_\pi \int d^4x\, d^4y\, e^{-ipx+ip'y} \langle \pi | \bar{q}(y) q(x) O_6(0)\rangle \\ &\underset{p,p'\to\infty}{\sim} \int d^4x\, d^4y\, e^{-ipx+ip'y} c_W(x,y) \langle \pi | \bar{q}\gamma_5 q(0)\rangle\,, \end{aligned} \tag{72}$$

where f_π is pion decay constant. The first equality in Eq. (72) follows from PCAC, the second from inserting the leading non-vanishing contribution of the O.P.E.

$$\bar{q}(y) q(x) O_6(0) \underset{x\sim y\sim 0}{\sim} c_W(x,y) \bar{q}\gamma_5 q(0) + \dots\,. \tag{73}$$

A straightforward dimensional argument leads to the asymptotic scaling law

$$c_W(\lambda p, \lambda p') = \int d^4x\, d^4y\, e^{-i\lambda px + i\lambda p'y} c_W(x,y) \underset{\lambda\to\infty}{\sim} \lambda^{-2}\,. \tag{74}$$

The trouble with this behaviour is that it is the same as that predicted by Eq. (69) for an operator of dimension $d = 3$. This simple observation proves our theorem. In fact, in the "kinematical" situation of the example we are considering, it would be impossible to distinguish at high momenta the contribution to the axial WTI coming from an operator of dimension 3 from the similar one due to the exchange of a massless pion in G_6^m.

Appendix B

In this appendix we wish to give a simple argument to show that in a gauge-fixed theory BRST symmetry does not forbid the mixing of gauge invariant operators with gauge non-invariant ones if the latter vanish by the equations of motion [22, 23].

To simplify notations we collectively indicate by $[\phi_k(x)]$ the set of fundamental (fermionic and bosonic) fields, including ghosts, appearing in the Lagrangian of the theory and by $[B_k(x)]$ their (bosonic and fermionic) BRST variations [8]:

$$\delta_{\rm B}\phi_k(x) = B_k(x)\,. \tag{75}$$

Introducing the sources $J^k_B(x)$, coupled to the variations $B_k(x)$, we define the so-called Zinn-Justin functional by

$$\begin{aligned}\mathcal{Z}[j, J_B, \eta] &\equiv \int \mathcal{D}\phi\, \exp\{-\mathcal{S}[\phi] + \int \phi_k j^k + \int J^k_B B_k + \int \eta O\} \equiv \\ &\equiv \int \mathcal{D}\phi\, \exp\{\mathcal{A}[\phi, J_B] + \int \phi_k j^k + \int \eta O\}\,,\end{aligned} \tag{76}$$

where η is the source coupled to the BRST-invariant operator O and a summation over repeated indices is understood. Expectation values with respect to this measure will be denoted

$$\langle\rangle\,\Big|_{j,J_B,\eta}\,. \tag{77}$$

In the second equality of Eq. (76) we have introduced the definition

$$\mathcal{A}[\phi, J_B] \equiv -\mathcal{S}[\phi] + \int J^k_B B_k\,. \tag{78}$$

We assume that the operator O is renormalized, so that its insertions with the fundamental fields of the theory are finite if the fields and O are physically separated. The issue at hand is whether there can be contact terms, whose coefficients diverge when the regularization is removed, and the removal of which requires the use of gauge non-invariant operators.

All the consequences of the BRST symmetry can be compactly expressed by the so-called Zinn-Justin equation

$$\int dx \frac{\delta \mathcal{Z}[j, J_B, \eta]}{\delta J^k_B(x)} j^k(x) = 0\,. \tag{79}$$

This is derived by performing the change of variables induced by the BRST transformations (75) in the functional integral (76), assuming that the Jacobian is unity. It is useful to expose the condition on B_k that a unit Jacobian implies:

$$\begin{aligned} 0 &= \int dx \int \mathcal{D}\phi\, \frac{\delta}{\delta\phi_k(x)} \Big\{ B_k(x) \exp\{\mathcal{A}[\phi, J_B] + \int \phi_k j^k + \int \eta O\} \Big\} \\ &= \left\langle \int dx \frac{\delta B_k(x)}{\delta \phi_k(x)} \right\rangle \Big|_{j,J_B,\eta} + \left\langle \int dx B_k(x) j_k(x) \right\rangle \Big|_{j,J_B,\eta} \end{aligned} \tag{80}$$

[8] Throughout this appendix to avoid cumbersome equations we will be rather cavalier about signs.

where we have used the BRST invariance of the action,

$$0 = \delta_{\rm B}\mathcal{S} = \int dx B_k(x) \frac{\delta \mathcal{S}}{\delta \phi_k(x)}\,, \tag{81}$$

and the nilpotency of BRST transformations,

$$0 = \int dy B_j(y) \frac{\delta B_k(x)}{\delta \phi_j(y)}\,. \tag{82}$$

The Zinn-Justin equation (79) follows from (80) as long as the condition for unit Jacobian,

$$\left\langle \int dx \frac{\delta B_k(x)}{\delta \phi_k(x)} \right\rangle \Big|_{j,J_B,\eta} = 0\,, \tag{83}$$

is satisfied. One readily verifies that antisymmetry arguments imply that this equation is trivially satisfied. Indeed, the BRST variations, B_k, are such that

$$\frac{\delta B_k(x)}{\delta \phi_k(x)} \equiv 0\,. \tag{84}$$

We note that the Zinn-Justin equation holds in a regularized theory as long as regularized BRST transformations can be defined under which the regularized action is invariant, and which satisfy (83). This is the case for lattice QCD [24](see sec. 2.1).

The regularized Green functions of the operator O obey the Slavnov-Taylor identities that follow from Eq. (79). If these Green functions contain contact terms which diverge when the regulator is removed, then these contact terms must separately satisfy the identities. Thus we can choose the counter-terms we add to cancel these divergences so that the identities, and thus the Zinn-Justin equation itself, are still satisfied. Thus we introduce the modified functional

$$\widetilde{\mathcal{Z}}[j, J_B, \eta] \equiv \int \mathcal{D}\phi \, \exp\{\mathcal{A}[\phi, J_B] + \int \phi_k j^k + \int \eta (O + F[J_B, \phi])\}\,, \tag{85}$$

where $F[J_B, \phi]$ is a local functional of the sources, J_B^k, and the fundamental fields, ϕ_k, and derive the constraints imposed on the form of the functional F by the modified Zinn-Justin equation

$$\int dx \frac{\delta \widetilde{\mathcal{Z}}[j, J_B, \eta]}{\delta J_B^k(x)} j^k(x) = 0\,. \tag{86}$$

The significance of the dependence of F on J_B^k will become apparent in the concrete example we give below.

A little calculation shows that (86) is equivalent to the equation

$$\begin{aligned} &\Big\langle \int dy\, \eta(y) \Big[\int dx \frac{\delta^2 F(y)}{\delta J_B^k(x) \delta \phi_k(x)} + W F(y) \Big] + \\ &+ \int dy\, \eta(y) \int dy' \eta(y') \int dx \frac{\delta F(y)}{\delta J_B^k(x)} \frac{\delta (O(y') + F(y'))}{\delta \phi_k(x)} \Big\rangle \Big|_{j,J_B,\eta} = 0\,, \end{aligned} \tag{87}$$

where we have introduced the operator

$$W = \int dx \Big(\frac{\delta \mathcal{A}}{\delta \phi_k(x)} \frac{\delta}{\delta J_B^k(x)} + \frac{\delta \mathcal{A}}{\delta J_B^k(x)} \frac{\delta}{\delta \phi_k(x)} \Big) =$$
$$= \int dx \Big(\frac{\delta \mathcal{A}}{\delta \phi_k(x)} \frac{\delta}{\delta J_B^k(x)} + B_k(x) \frac{\delta}{\delta \phi_k(x)} \Big) , \tag{88}$$

so that

$$WF(x) = \int dy \frac{\delta \mathcal{A}}{\delta \phi_k(y)} \frac{\delta F(x)}{\delta J_B^k(y)} + \delta_{\rm B} F(x) . \tag{89}$$

To get Eq. (87) we have exploited the identity (84) and the BRST-invariance of the generalized action (Eq. (78)), which in our notation amounts to the two equations (81) and (82). Limiting for simplicity the analysis to Green functions with single insertions of the operator O, Eq. (87) implies the condition

$$WF(x) + \hbar \int dy \frac{\delta^2 F(x)}{\delta \phi_k(y) \delta J_B^k(y)} \equiv W' F(x) = 0 , \tag{90}$$

where we have reinstated the dependence on $\hbar$, and defined the new operator W'.

The key observation needed to solve (90) is to recognize [22] that W is a nilpotent operator, $W^2 = 0$. Using this property, and the fact the fermionic operator $\int dy \delta^2 / \delta J_B^k(y) \delta \phi_k(y)$ is nilpotent, it then follows that W' itself is nilpotent, $W'^2 = 0$. Thus a solution to (90) is $F = W'C$. To show that this is the only solution, to all orders in perturbation theory, we expand F in powers of $\hbar$: $F = F_0 + \hbar F_1 + \hbar^2 F_2 + \hbar^3 F_3 + \ldots$. Introducing this expansion in Eq. (90) and repeatedly using the nilpotency of W and W', one obtains the solution in the form[9]

$$F = W(C_0 + \hbar C_1 + \hbar^2 C_2 + \hbar^3 C_3 + \ldots) +$$
$$+ \hbar \int dy \frac{\delta^2}{\delta \phi_k(y) \delta J_B^k(y)} (C_0 + \hbar C_1 + \hbar^2 C_2 + \ldots) , \tag{91}$$

where $C_i[\phi, J_B]$ are arbitrary local functionals of the sources, J_B, and the fundamental fields of the theory. The series expansion in $\hbar$ in the r.h.s. of Eq. (91) can be formally resummed, giving

$$F(x) = W'C(x) = WC(x) + \hbar \int dy \frac{\delta^2 C(x)}{\delta \phi_k(y) \delta J_B^k(y)} . \tag{92}$$

Remembering the form of W (see Eq. (88)), we can split F in a BRST-invariant and a non BRST-invariant part:

$$F(x) = F_{NB}(x) + \delta_{\rm B} C(x) \tag{93}$$

$$F_{NB}(x) = \int dy \frac{\delta A}{\delta \phi_k(y)} \frac{\delta C(x)}{\delta J_B^k(y)} + \hbar \int dy \frac{\delta^2 C(x)}{\delta \phi_k(y) \delta J_B^k(y)} . \tag{94}$$

[9] To begin the iteration one needs the result that solutions to $WG = 0$ are of the form $G = WH$, where H is a local functional of fields and sources [22].

We are really interested in F_{NB}, because the BRST-invariant part of F can always be reabsorbed in a redefinition of O. We can now see that, as expected, the insertion of F_{NB} with the fundamental fields of the theory gives rise only to contact terms, thanks to the locality of the functional C. To see this we consider the Green function

$$\begin{aligned} &G(x, x_1, \ldots, x_n) = \\ &= \int \mathcal{D}\phi \, \mathrm{e}^{\mathcal{A}[\phi, J_B]/\hbar} F_{NB}(x) \phi_{k_1}(x_1) \ldots \phi_{k_n}(x_n) \, . \end{aligned} \tag{95}$$

Inserting Eq. (94) one gets, after an integration by parts,

$$\begin{aligned} &G(x, x_1, \ldots, x_n) = \\ &= -\hbar \sum_{i=1}^{n} \delta(x - x_i) \, \langle \phi_{k_1}(x_1) \ldots X_{k_i}(x_i) \ldots \phi_{k_n}(x_n) \rangle \ , \end{aligned} \tag{96}$$

where we have used the definition

$$\frac{\delta C(x)}{\delta J_B^{k_i}(x_i)} \equiv X_{k_i}(x) \delta(x - x_i) \, . \tag{97}$$

If we now set $J_B = 0$ in Eq. (96) we see explicitly that F_{NB} generates contact terms, and that they are not constrained by BRST symmetry (since C and thus the X_k are arbitrary).

Returning to the full expression of F, we can now rewrite Eq. (92) as

$$F(x) = \frac{\delta \mathcal{A}}{\delta \phi_k(x)} X_k(x) + \delta_{\mathrm{B}} C(x) + \hbar \frac{\delta X_k(x)}{\delta \phi_k(x)} \, . \tag{98}$$

Apart from the last term, Eq. (98) proves our initial statement, i.e. F vanishes by the equations of motion up to BRST-invariant terms. The last term is proportional to $\delta(0)$. It is present to ensure that the term vanishing by the equations of motion does in fact lead to a contact term [as seen in the derivation of Eq. (96) above]. More formally, it compensates divergent contact terms (hidden) in the product of operators appearing in the first term of Eq. (98). For the flavor non-singlet operators considered in this work, one can in fact show that this term is algebraically zero.

We want to end this appendix by clarifying, in a significant example, the physical meaning of the presence of the counter-term F in Eq. (85). For this purpose let us consider the Slavnov-Taylor identity

$$\Big[\frac{\delta^3 \widetilde{\mathcal{Z}}}{\delta j^n(z) \delta J_B^m(t) \delta \eta(x)} + \frac{\delta^3 \widetilde{\mathcal{Z}}}{\delta j^m(t) \delta J_B^n(z) \delta \eta(x)} \Big] \Big|_{j = J_B = \eta = 0} = 0 \, , \tag{99}$$

that follows from equation (86) by successively differentiating with respect to $j_m(t)$, $j_n(z)$ and $\eta(x)$. After some algebra one gets [10]

$$\frac{\delta^3 \widetilde{\mathcal{Z}}}{\delta j^n(z) \delta J_B^m(t) \delta \eta(x)} \Big|_{j = J_B = \eta = 0} = \langle \phi_n(z) B_m(t) O(x) \rangle + \tag{100}$$

[10] To avoid introducing a new symbol we now use X_k to indicate the functional derivative $\delta C / \delta J_B^k$ *evaluated at* $J_B = 0$.

$$+\delta(x-z)\,\langle X_n(z)B_m(t)\rangle + \delta(x-t)\,\langle \phi_n(z)\delta_{\rm B}(X_m(t))\rangle + \\ +\delta(x-z)\delta(x-t)\,\langle X_{nm}(x)\rangle$$

$$\left.\frac{\delta^3\widetilde{\mathcal{Z}}}{\delta j^m(t)\delta J_B^n(z)\delta\eta(x)}\right|_{j=J_B=\eta=0} = \langle \phi_m(t)B_n(z)O(x)\rangle + \\ +\delta(x-t)\,\langle X_m(t)B_n(z)\rangle + \delta(x-z)\,\langle \phi_m(t)\delta_{\rm B}(X_n(z))\rangle + \\ +\delta(x-z)\delta(x-t)\,\langle X_{mn}(x)\rangle\ . \tag{101}$$

In the above equations we have used the formal expansion [11]

$$C(x) = \sum_{n=1}^{\infty} J_B^{k_1}(x)\ldots J_B^{k_1}(x)X_{k_1\ldots k_n}(x)\,. \tag{102}$$

In Eqs. (100) and (101) we see explicitly the meaning of the terms in F_{NB} proportional to J_B (which arise in part from terms in C quadratic in J_B): they lead to the double contact terms proportional to X_{nm}. Notice that the sum of all contact terms adds up to zero by itself by virtue of the (anti)symmetry properties of X_{nm} and of the BRST identity obeyed by $\langle B_n(z)X_m(t)\rangle$, which reads

$$\langle X_m(t)B_n(z)\rangle = \langle \delta_{\rm B}(\phi_n(z))X_m(t)\rangle = -\,\langle \phi_n(z)\delta_{\rm B}(X_m(t))\rangle\ . \tag{103}$$

The cancellation of contact terms is also consistent with the equation

$$\langle B_m(t)\phi_n(z)O(x)\rangle + \langle \phi_m(t)B_n(z)O(x)\rangle = \langle \delta_{\rm B}(\phi_m(t)\phi_n(z)O(x))\rangle = 0 \tag{104}$$

that follows from the BRST invariance of O.

Let us summarize what we have learned. It is consistent with BRST invariance for the gauge-invariant operator to have (divergent) contact terms with the fundamental fields. These can be cancelled by appropriate choices of the X_n and X_{nm} in such a way that the resulting correlation functions have finite Fourier transforms. In other words, adding the counter-term F amounts to redefining the correlation functions as follows:

$$\langle \phi_m(t)B_n(z)O(x)\rangle' \equiv \langle \phi_m(t)B_n(z)O(x)\rangle + \\ +\delta(x-z)\,\langle \phi_m(t)\delta_{\rm B}(X_n(z))\rangle + \delta(x-t)\,\langle X_m(t)B_n(t)\rangle + \\ +\delta(x-z)\delta(x-t)\,\langle X_{mn}(x)\rangle\ , \tag{105}$$

so that they are finite for all x, z and t. The Slavnov-Taylor identity (99) then implies that

$$\langle \phi_m(t)B_n(z)O(x)\rangle' + \langle \phi_n(z)B_m(t)O(x)\rangle' = 0\,, \tag{106}$$

i.e. $\langle \phi_m(t)B_n(z)O(x)\rangle'$ and $\langle \phi_m(t)B_n(z)O(x)\rangle$ satisfy the same BRST identity.

[11] The term with $n = 0$ is dropped from the expansion because a J_B-independent piece would give a BRST-invariant contribution to O.

What are the constraints on the counter-term implied by BRST invariance? Although X_n, the contact term between ϕ_n and O, is not constrained, the contact term between $\delta_B\phi_n$ and O is required to be $\delta_B X_n$. This relationship between contact terms is encoded in the J_B dependence of F. If more than two fields collide, then additional arbitrary contact terms are allowed. This way of understanding the result makes it clear that the general form of the contact terms could, with a lot of imagination, have been guessed without reference to the Zinn-Justin equation.

Appendix C

In this appendix we test our method for off-shell improvement using one-loop perturbation theory. We focus on the quark propagator, the improvement of which requires, we claim, the gauge non-invariant term proportional to c_{NGI}. The necessary one-loop perturbative calculations have been worked out by Capitani *et al*, and presented in final form in Ref. [27]. We stress, however, that the method of off-shell improvement presented in Ref. [27] does not include the c_{NGI} term. It works, however, up to one-loop, because, as we shall show in this Appendix, c_{NGI} actually vanishes at tree-level.

It is convenient to work with the inverse bare lattice propagator since this is the quantity calculated in perturbation theory. Thus we rewrite Eq. (27) as

$$\frac{\widehat{S}^{-1}(p)}{Z_q^0} = S_L^{-1}(p)\left(1 + ab_q m - 2ac'_q S_L^{-1}(p) - 2ac_{\rm NGI} i\not{p} + {\rm O}(a^2)\right) . \tag{107}$$

Here we have used the fact that $[S_L^{-1}, \not{p}] = 0$ (since the only gamma-matrix structure allowed in S_L^{-1} is $\not{p}$), and expanded the quark-field normalization factor in the conventional way

$$Z_q = Z_q^0(1 + ab_q m) . \tag{108}$$

The advantage of moving Z_q^0 to the l.h.s. of Eq. (107) is that it separates the issues of improvement and normalization. The l.h.s. is proportional, up to $O(a^2)$, to the continuum inverse propagator, and thus it should be possible to choose b_q, c'_q and c_{NGI} so that the r.h.s. does not contain $O(a)$ terms. An important constraint is provided by the fact that these three improvement coefficients should be functions only of the bare coupling g_0^2.[12]

The one-loop result for the inverse propagator with an improved action takes the form

$$S_L^{-1}(p) = i\not{p} + m + \frac{ap^2}{2} - \lambda\Sigma_L + O(a^2) , \tag{109}$$

$$\Sigma_L = i\not{p}\Sigma_{1L} + m\Sigma_{2L} + ap^2\Sigma_{3L} + ai\not{p}m\Sigma_{4L} + am^2\Sigma_{5L} + \frac{i\not{p}m^2}{p^2}\Sigma_{6L} , \tag{110}$$

$$\lambda = \frac{g_0^2 C_F}{16\pi^2} , \tag{111}$$

[12]Strictly speaking, improvement coefficients are functions of the coupling $g_0^2(1 + b_g am)$, as explained in Ref. [7]. This distinction is, however, important only at two-loop order for the quark propagator.

where explicit results for the Σ_{jL} (for arbitrary m^2/p^2) can be deduced from the results in Ref. [27]. Here the quark mass is defined as usual

$$am = \frac{1}{2\kappa} - \frac{1}{2\kappa_c}\,, \tag{112}$$

using the one-loop result for κ_c. We need only the large p behavior of the Σ_{jL},

$$\Sigma_{jL} = \ell_j \ln(a^2p^2) + d_j + O(m^2/p^2)\,. \tag{113}$$

The coefficients of the logarithm are (using the appropriate leading order value, $c_{SW} = 1$)

$$\ell_1 = \ell_3 = \alpha\,, \quad \ell_2 = -\ell_4 = -2\ell_5 = (3+\alpha)\,, \quad \ell_6 = 0\,, \tag{114}$$

where α is the gauge parameter which vanishes in Landau gauge. It is important to note that subleading terms proportional to (m^2/p^2) are absent from Σ_{1L} and Σ_{3L}, since these are explicitly included in Σ_{6L} and Σ_{5L}, respectively. These terms do contribute in the large p^2 limit. However, the other such terms (in Σ_{2L} and $\Sigma_{4L} - \Sigma_{6L}$) give vanishing contributions in this limit.[13]

Using these results, we can evaluate the r.h.s. of Eq. (107)

$$\begin{aligned}
&\frac{\widehat{S}^{-1}(p)}{Z_q^0} = i\,\not{p}(1-\lambda\Sigma_{1L}) + m(1-\lambda\Sigma_{2L}) \\
&+ ap^2\left[2c'_q(1-2\lambda\Sigma_{1L}) + 2c_{NGI}(1-\lambda\Sigma_{1L}) + 1/2 - \lambda\Sigma_{3L}\right] \\
&+ ai\,\not{p}m\left[-4c'_q(1-\lambda\Sigma_{1L}-\lambda\Sigma_{2L}) - 2c_{NGI}(1-\lambda\Sigma_{2L}) + b_q(1-\lambda\Sigma_{1L}) - \lambda\Sigma_{4L}\right] \\
&+ am^2\left[-2c'_q(1-2\lambda\Sigma_{2L}+2\lambda\Sigma_{6L}) + b_q(1-\lambda\Sigma_{2L}) - c_{NGI}2\lambda\Sigma_{6L} - \lambda\Sigma_{5L}\right] + O(a^2,\lambda^2)\,.
\end{aligned} \tag{115}$$

From this we can deduce the constraints on the improvement coefficients. First we note that, for large momenta,

$$S^{-1}(p) = \widehat{S}^{-1}(p) + O(a^2) = -\frac{1}{p^2\Sigma_1(p^2)}\left(i\,\not{p} - \frac{\Sigma_2(p^2)}{\Sigma_1(p^2)}\right) + O(m_q^2/p^2)\,, \tag{116}$$

where we have used Eqs. (23) and (26). Asymptotically, $\Sigma_1(p^2)$ is independent of m_q, while $\Sigma_2/\Sigma_1 = m_q$ up to logarithmic corrections in p^2. It follows that, asymptotically, there are no terms proportional to p^2 and $i\,\not{p}m$ in $\widehat{S}^{-1}$, and so the coefficients of these terms in Eq. (115) must vanish. These constraints can be written (up to corrections of $O(\lambda^2)$)

$$2c'_q + 2c_{NGI} + 1/2 = \lambda\left[(4c'_q + 2c_{NGI} + 1)\Sigma_{1L} + (\Sigma_{3L} - \Sigma_{1L})\right]\,, \tag{117}$$

$$4c'_q + 2c_{NGI} - b_q = \lambda\left[(4c'_q - b_q)\Sigma_{1L} + (4c'_q + 2c_{NGI} + 1)\Sigma_{2L} - (\Sigma_{2L} + \Sigma_{4L})\right]\,. \tag{118}$$

The final constraint is obtained by noting that $\widehat{S}^{-1}$ depends linearly on the renormalized mass m_q, which is related to the lattice quark mass by

$$m_q = Z_m m(1 + ab_m m)\,. \tag{119}$$

[13] We thank Paul Rakow for pointing out to us the importance of including the apparently subleading form factor Σ_{6L}, as has been done in Ref. [27].

It follows that the ratio of m^2 and m terms in Eq. (115) gives b_m. In this way one finds

$$b_m + 2c'_q - b_q = \lambda\left[(2c'_q + 1/2)\Sigma_{2L} - (4c'_q + 2c_{NGI})\Sigma_{6L} - (\Sigma_{2L}/2 + \Sigma_{5L})\right] + O(\lambda^2)\,. \quad (120)$$

The three equations (117), (118) and (120) provide non-trivial constraints because their l.h.s.'s are constants, independent of ap, while the r.h.s.'s contain terms with logarithmic dependence on ap. At first sight, the system is over-constrained, because each of the three equations has an $O(1)$, an $O(g_0^2)$, and $O(g_0^2 \ln(ap))$ part, providing nine constraints in total, while there are four improvement constants, each with an $O(1)$ and an $O(g_0^2)$ part to be determined. It turns out, however, that the constraints are redundant, and, in fact, the system is under-constrained.

To proceed we expand the improvement constants in powers of λ, e.g.[14]

$$b_q = b_q^{(0)} + \lambda b_q^{(1)} + O(\lambda^2)\,. \quad (121)$$

Then the first constraints are that the l.h.s.'s of the three equations vanish at leading order, since the r.h.s.'s are of $O(\lambda)$. This gives

$$2c'^{(0)}_q + 2c^{(0)}_{NGI} + 1/2 = 0\,, \quad 4c'^{(0)}_q + 2c^{(0)}_{NGI} - b^{(0)}_q = 0\,, \quad b^{(0)}_m + 2c'^{(0)}_q - b^{(0)}_q = 0\,. \quad (122)$$

We see that, as noted in the text, we cannot determine the tree-level value of all four constants with a tree-level computation of the propagator. Only the combinations $c'^{(0)}_q + c^{(0)}_{NGI} = -1/4$, $2c'^{(0)}_q - b^{(0)}_q = 1/2$ and $b^{(0)}_m = -1/2$ are determined.

The one-loop computation does, however, completely determine the tree-level improvement coefficients. To see this, note that we have written the three equations so that the combination of Σ_{jL} in the last term on each r.h.s. has no dependence on $\ln(a^2p^2)$ [see Eq. (114)], and is thus just a constant (in any covariant gauge). In Landau gauge, Σ_{1L} is also a constant, but Σ_{2L} has a logarithmic part. To cancel this logarithmic part on the r.h.s.'s of Eqs. (118) and (120) requires

$$4c'^{(0)}_q + 2c^{(0)}_{NGI} + 1 = 0\,, \qquad 2c'^{(0)}_q + 1/2 = 0\,. \quad (123)$$

These two extra equations could be inconsistent with the previous three, and is a non-trivial test of improvement that they are not. They provide the extra constraint needed to determine the tree level improvement coefficients, and one finds that

$$c^{(0)}_{NGI} = 0\,. \quad (124)$$

Thus the "new" constant does vanish at tree level, but from the point of view of the calculation this is an accident. For the tree-level values of the other two constants one finds $c'^{(0)}_q = -1/4$ and $b^{(0)}_q = 1$.

We note in passing that the coefficient of Σ_{1L} in Eq. (117) does vanish due to Eq. (123). This means that the improvement works in perturbation theory at one-loop in any covariant gauge.

[14]Note that it is standard to expand in powers of g_0^2 rather than λ. We choose to expand in λ so as to simplify equations.

Finally, we can deduce the constraints from the non-logarithmic $O(\lambda)$ terms. These can be written

$$2c_q'^{(1)} + 2c_{NGI}^{(1)} = \Sigma_{3L} - \Sigma_{1L} \,, \tag{125}$$

$$2c_q'^{(1)} - b_q^{(1)} = -\Sigma_{3L} + \Sigma_{1L} - \Sigma_{2L} - \Sigma_{4L} \,, \tag{126}$$

$$b_m^{(1)} = \Sigma_{3L} - \Sigma_{1L} + \Sigma_{2L}/2 + \Sigma_{4L} - \Sigma_{5L} + \Sigma_{6L} \,. \tag{127}$$

Thus a one-loop computation of the propagator does not determine $c_{NGI}^{(1)}$. To do so would require a two-loop computation of the propagator. Alternatively, noting that the gauge non-invariant term can be rewritten as $\not{A}q$, it seems likely that a one-loop computation of the quark-gluon vertex would determine $c_{NGI}^{(1)}$.

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